

Edge States in Doped Antiferromagnetic Nano-Structures

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We study competition between different phases in a strongly correlated nano-structure with an edge. Making use of the self-consistent Green's function and density matrix renormalization group methods, we study a system described by the t - J_z and t - J models on a strip of a square lattice with a linear hole density $n_{||}$. At intermediate interaction strength J/t we find edge stripe-like states, reminiscent of the bulk stripes that occur at smaller J/t . We find that stripes attach to edges more readily than hole pairs, and that the edge stripes can exhibit a peculiar phase separation.

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It is well established by now that in the ground state of the two-dimensional (2D) strongly correlated cuprates, much studied in the context of the high- T_c problem,^{1,2} charge carriers tend to be distributed inhomogeneously. Such inhomogeneities occur as an attempt to reduce the frustration between the exchange and kinetic energies arising from the antiferromagnetic (AF) background.¹ It is conceivable that such frustration can be further reduced at a boundary. This would induce an effective attraction of the bulk inhomogeneity to the edge, thus leading to a novel, many-body type edge state. A bulk doped Mott insulator might have various types of striped, paired, or unpaired ground states. Ordinarily one is not concerned with surface states. However, for cuprate nanoscale structures, which are of interest due to recent progress in nano-synthesis,³ one may potentially have a system with a finite doping in which the holes are bound to the edges. In this case, understanding the possible edge states is crucial.

Here, we consider the simplified case of a half-plane, or similarly, one end of a long open cylinder, with a vanishingly small doping sufficient to form a finite *linear* concentration $n_{||} = N_h/L$ of holes near the edge. N_h is the number of holes and L is the linear size of the system. Given this configuration, several questions arise. For example, if the holes form a single stripe in the bulk, does this stripe attach itself to the edge? Do single pairs attach to the edge? Can one have a one-dimensional (1D) "edge phase separation" with the holes clustered together in edge droplets?

In this paper we address some of these questions in the context of the t - J_z and t - J models, using the self-consistent Green's function and the density matrix renormalization group (DMRG) methods. We obtain an approximate edge phase diagram in which the linear hole density $n_{||}$ is a control parameter. We find analytically, for the t - J_z model, that the stripe edge states do exist in a substantial region of the phase diagram. This is verified for both the t - J_z and t - J models using DMRG for systems up to 11×8 sites with periodic/open and 20×5 with open boundary conditions. We also find that the Ising anisotropy enhances tendency to the edge states formation. A remarkable feature of these states is that they are

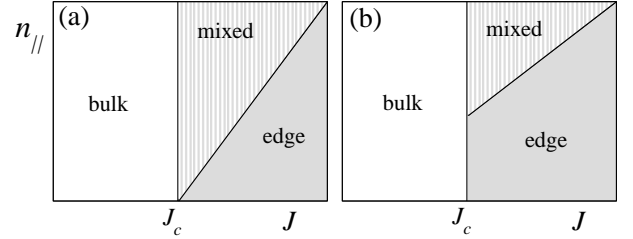


FIG. 1: Phase diagram of a system with an edge, in the linear hole concentration ($n_{||}$) v.s. attraction to the edge (J) plane. (a) band-like case, (b) case of complex bulk/edge states. The labels of the phases indicate where the holes reside.

reminiscent of and, as we show in some detail, are directly related to the bulk stripe states observed in the studies of strongly correlated models as well as in real high- T_c materials.^{1,2,4} We argue that such edge states can be a common feature of strongly correlated nano-systems.

With our Fig. 1 we outline two generic possibilities for the formation of the edge state as a function of attraction to the boundary (controlled by J) and linear hole concentration $n_{||}$. Fig. 1(a) corresponds to the case when both the 2D bulk and the 1D edge state are band-like. At small J the kinetic energy in the bulk is lower and the holes occupy the bulk states only (bulk). At $J = J_c$ the bottom of the edge-band becomes degenerate with the bulk band. As the attraction to the edge is increased further, a fraction of holes from the bulk populates the edge band (mixed). Upon the further increase of J all the holes are in the edge band (edge). Note that in the bulk and mixed states the chemical potential is pinned at the bottom of the bulk band as the finite linear concentration $n_{||} = N_h/L$ corresponds to zero bulk concentration $x = N_h/L^2$, as $L \rightarrow \infty$. Fig. 1(b) outlines a different generic scenario in which the edge state formed at $J = J_c$ accumulates a finite linear concentration of holes. That is, at J_c a finite amount of holes $n_{||}^c$ becomes attached to the boundary at once. This could occur, for example, if the lowest energy state is a stripe attached to the edge.

In this work we focus on a particular case of the strongly correlated models, the t - J_z and the t - J models,

and, therefore, on a particular case of such a frustration characteristic to the doped antiferromagnets. We find, by means of analytical and numerical approaches, that the edge states do form in these systems and that their phase diagram belongs to the class described in Fig. 1(b).

First, we provide a general reasoning for the edge states to occur in the t - J -like models. Excitations in such models doped with few holes are described as spin-polarons, which either form moderately bound pairs or move independently.⁴ It is clear that at some J/t such excitations would reside close to an edge where they frustrate the AF background less. Thus, edge holes or edge pairs can be formed. At larger densities the holes are known to be in the “bulk” quasi-1D stripes with internal hole concentration close to $n_{\parallel} = 1/2$.⁴ Although the kinetic energy advantage for holes in the stripe is substantial, the magnetic energy cost of the antiphase-domain wall (ADW) associated with the stripe is considerable too, $E_{mag} \sim J$ per hole. However, this magnetic energy of the domain wall can be significantly reduced at the edge. Therefore, an edge stripe can be formed. One may also expect that the low-density stripes will be attracted to the edge more readily because their magnetic energy is higher ($E_{mag} \sim J/n_{\parallel}$) and its reduction should be more effective for them. Thus, one expects that in some range of n_{\parallel} and J an edge stripe can be formed.

Note that within this scenario edge stripes constitute many-body states formed due to a non-trivial collective effect. That is, the energy is reduced due to attraction of the stripe as an entity. This means that if the ground state of the t - J model would be given by a dilute gas of spin polarons then the physics outlined in Fig. 1(a) should be applicable to the bulk and edge bands of these excitations. However, if the ground state is a stripe, then we expect the edge phase diagram of Fig. 1(b).

Another important question here is: what is the ground state of the t - J model in the limit of small $n_{\parallel} \ll 1/2$? The most likely answer is that the ground state is given by a closed “stripe loop” with an AF antiphase shift across the loop and internal hole concentration close to the “optimal” $n_{\parallel} = 1/2$, as supported by the observation in our previous work, Ref. 4. Such loops can be seen as nucleations of the “straight” stripes. In this regime we expect the edge states to consist of short loop-like segments.

To demonstrate the described tendencies explicitly and quantitatively we consider the t - J model:

$$\mathcal{H} = -t \sum_{ij,\sigma} \tilde{c}_{i\sigma}^{\dagger} \tilde{c}_{j\sigma} + \frac{J}{2} \sum_{ij} \left(\mathbf{S}_i \cdot \mathbf{S}_j - \frac{n_i n_j}{4} \right), \quad (1)$$

on a strip of a square lattice and in the standard notations of constrained fermion and spin operators, J is the superexchange and t is the kinetic energy, and summation is over nearest-neighbor sites.

First, we consider a simpler problem where we impose a local constraint on the linear hole density. Namely, a given n_{\parallel} will be assumed to be distributed homogeneously along the boundary. This consideration will help

to clarify the details of the competition between different bulk and edge states such as a dilute gas of holes/pairs and “straight” stripes, but will exclude the 1D phase separated states such as loops. In reality, such a constraint may be imposed by the confinement effect of finite sizes of a structure or by extra interactions beyond the considered models. In a nano-size system single-hole and single-pair states can be of interest themselves.

We will be mostly concerned with the study of the anisotropic version of the model, the t - J_z model, for which the bulk stripe, pairing, and Nagaoka states, very similar to those of the isotropic t - J model, have been found in the past.^{4,5} One can argue that the t - J_z model should reproduce qualitatively the holes’ ground state of the isotropic t - J model, although the details of such states might differ. Moreover, for the bulk stripe phase in this model a very close *quantitative* agreement between the analytical and numerical methods have been demonstrated in our previous work.⁴ Here we provide an extensive analysis of the stripes and other excitations of the model (1) in the presence of the boundaries.

The stripe occurs due to the lowering of the kinetic energy of holes at the 1D ADW. Although the stripe is always beneficial from the point of view of kinetic energy, there is a magnetic energy of the ADW, $\sim L J_z$, which one needs to compensate. Ignoring hole-hole interaction the energy of the bulk stripe is given by:

$$\frac{E_{total}}{N_h} = \frac{J_z}{2} (n_{\parallel}^{-1} - 1) + (\pi n_{\parallel})^{-1} \int_0^{k_F} E_k dk, \quad (2)$$

where E_{total} is relative to E_0 of the hole-free Ising AF background, k is a 1D wave-vector along the stripe. The first term in (2) is the magnetic energy and the second term is the energy of the effective 1D band of holes filled up to the Fermi momentum $k_F = \pi n_{\parallel}$. The quasiparticle energy E_k is defined through the Dyson’s equation: $E_k + 2t \cos(k) - \Sigma(E_k) = 0$ where $\Sigma(\varepsilon)$ is the self-energy due to the string-like hole motion away from stripe. $\Sigma(\varepsilon)$ can be written in a compact form and Dyson equation can be solved numerically (see Ref. 4). The bulk stripe energy is shown in Fig. 2(a) as a function of n_{\parallel} for two representative J_z/t values (solid lines). There is an excellent agreement of the theory with the DMRG data for $J_z/t = 0.35$ in an 11×8 system (circles).

This bulk stripe energy should be compared to the one of bulk holes/pairs. In a homogeneous AF holes attract each other in a bound state with the binding energy E_b ($\simeq -J_z/2$ for $J_z/t \gg 1$ and $\sim -J_z^3/t^2$ for $J_z/t \ll 1$).⁵ For the dilute system we assume that the hole pairs do not overlap and $E_{total}^{pair} = N_h(E_{polaron} + E_b/2)$, shown by the straight lines in Fig. 2(a).

In the presence of the boundary two types of new states are possible, the edge pair and the edge stripe. Our calculations within the retraceable path approximation show that the transition from the bulk pair to the edge pair occurs at $J_z/t \approx 0.4$. For the edge stripe the longitudinal kinetic energy due to motion along the edge should

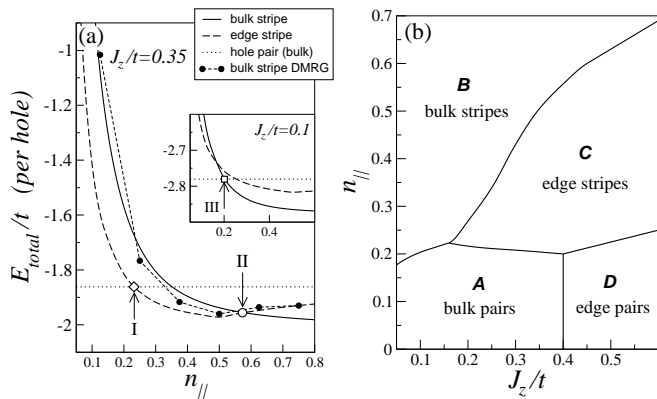


FIG. 2: (a) Energy of the system per hole as a function of hole density $n_{||}$ for the bulk and edge stripe, and the bulk pair state in the t - J_z model (solid, dashed, and dotted, respectively). Black circles are the DMRG data for the bulk stripe, Ref. 4. $J_z/t = 0.35$, and $J_z/t = 0.1$ (inset). Open symbols denote transitions: **I** - pair to edge stripe, **II** - edge to bulk stripe, **III** - pair to bulk stripe. (b) Constrained (see text) phase diagram of the t - J_z system with an edge. **A** - bulk pairs, **B** - bulk stripes, **C** - edge stripes, **D** - edge pairs.

remain the same as for the bulk stripe while the magnetic and transverse kinetic energy change. At the stripe the hole excitations correspond to geometric kinks in the magnetic domain wall.⁴ Therefore, placing the stripe at the edge eliminates one-half of the broken bonds in the ADW and the magnetic energy of the stripe is reduced to $J_z/2 (1/2n_{||} - 1)$ per hole. The transverse kinetic energy is modified too, which leads to a different form of the self-energy $\Sigma(\varepsilon)$ in the Dyson equation. As a result the total energy of the edge stripe is given by the same expressions as in Eq. (2) with the reduced magnetic energy and different $\Sigma(\varepsilon)$. The resulting E_{total}^{edge} are shown in Fig. 2(a) by the dashed lines. One can clearly see the $1/n_{||}$ behavior in the bulk and edge stripe energies at low $n_{||}$ where the magnetic energy dominates. For $J_z/t = 0.35$ the first transition, which occurs at a lower $n_{||} \approx 0.22$, is from the bulk pairs to the edge stripe state. At higher density $n_{||} \approx 0.58$ a transition to the bulk stripe occurs. For the smaller value of $J_z/t = 0.1$ the edge stripe never materializes in the ground state and the transition is only between the bulk stripe and bulk pairs state (Fig. 2(a), inset). Varying the values of J_z/t in such an analysis we obtain the “constrained” phase diagram in Fig. 2(b).

At small J_z/t the boundary is irrelevant and the competition is between the bulk striped and paired states only. At low $n_{||}$ stripes cannot be formed as $E_{mag} \propto J_z/n_{||}$ is too high. At intermediate J_z/t the edge stripes form readily, while it is only at larger J_z/t when the edge pairs are formed. Note that the pairs-to-stripes boundary in Fig. 2(b) is only weakly J_z/t -dependent. At larger J_z/t the boundary is between the edge stripes and edge pairs. In principle, there can be more subtle varieties of the quasi-1D states at the edge, including density-wave and others, which might be classified according to the

Luttinger liquid g -ology.⁶ Complicating such a classification is the bulk AF background breaking spin symmetry.

As J_z/t increases the edge state gets strongly attached to the boundary and the energy difference between the competing phases in this region becomes rather small. In that case, the qualitative distinctions between the edge pairs and edge stripes, such as the anti-phase shift of the AF order parameter across the stripe, diminishes and one is not able to tell what bulk state a given edge state is associated with. Thus, one can expect a crossover from the edge stripes to the edge pairs at larger J_z/t .

We have used DMRG to verify numerically the existence of these states.² We have studied systems $L_x \times L_y$ up to 11×8 sites, with periodic boundary conditions (BCs) in the L_y direction and open BCs in L_x direction (representing the edges). No external field was applied to the open boundaries.^{2,4} Altogether, we have a close agreement between our analytical and numerical results. All the principal phases, bulk and edge stripe, and bulk and edge pair states are identified. Because of the finite sizes of the modeled systems only a discrete set of hole densities $n_{||}$ is available, while J_z/t can be varied continuously. We have studied the clusters 11×4 with one hole, 11×6 with two holes, and 11×8 with two and four holes. The number of states kept ranged from 1000 to 4000, with as many as 20 sweeps, allowing each run to converge nicely. An evolution from the bulk to the edge stripe was observed in our 11×4 ($n_{||} = 0.25$) and 11×6 ($n_{||} = 0.33$) clusters. There we start from the bulk stripe at small J_z/t in the center of the cluster,⁴ which broadens and becomes degenerate with the edge stripe upon increase of J_z/t , and then forms the edge state, see Fig. 3(a). One can find remnants of the antiphase π -shift due to the ADW for the edge stripe in Fig. 3(a), a clear signature that this state remains quantum-mechanically connected to the bulk stripe. If, on the other hand, we start from the bulk paired state, (11×8 , two holes) we have a transition to an edge state at around $J_z/t = 0.4$ (in agreement with the analytical calculation), which has no stripe-like magnetic correlation and we classify it as the edge pair. Another distinction is the energy. One can compare the energies per hole of the systems of different size with the same number of holes in which the edge pair and the edge stripe are formed (11×6 and 11×8 with two holes). Generally, such per hole energies are lower in the edge stripe state, which indicates that: (i) the edge stripe is distinct from the edge pair, and that (ii) the edge state will be favored in the thermodynamic limit. Upon further increasing of J_z/t the energies of the edge states become degenerate as shown by such a comparison, which supports our suggestion of the crossover from the edge stripe to the edge pair state at larger J_z/t .

Also, for the concentration $n_{||} = 0.25$ we observe no transition from paired states to stripes as a function of J_z/t , in a close agreement with a flat boundary between pairs and stripes in our analytical results in Fig. 2(b).

Note here that we also found similar states in the case of the fully isotropic t - J model, with the phase bound-

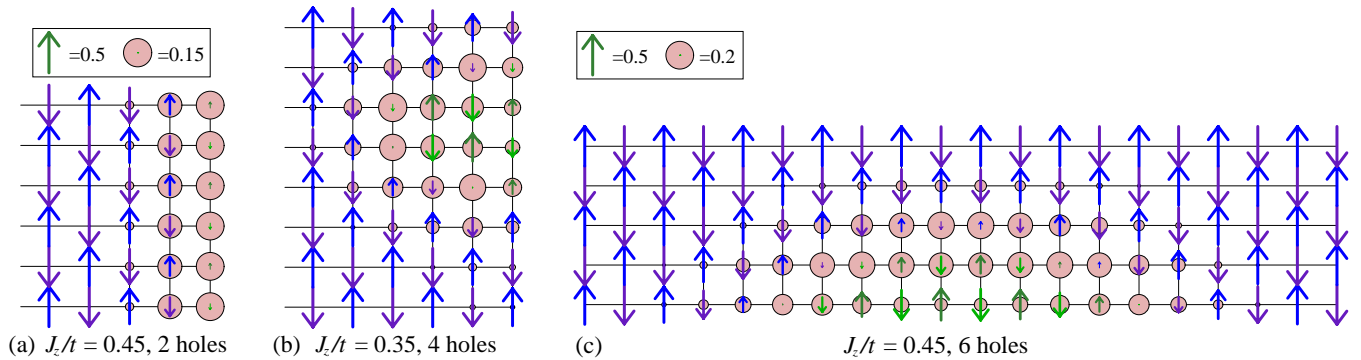


FIG. 3: DMRG results for the edge stripes in the t - J_z model in (a) 11×6 , (b) 11×8 , and (c) 20×5 clusters. J_z/t and the number of holes is as indicated. In (a) and (b) only the right half of the cluster containing all the holes is shown with the rightmost column being the open boundary. In (c) the bottom row is the “free” open boundary (see text). The arrows represent the on-site value of $\langle S_i^z \rangle$ and the circles are for the hole density $\langle n_i \rangle$. Scales for $\langle S_i^z \rangle$ and $\langle n_i \rangle$ in (b) and (c) are the same.

aries shifted to somewhat higher J/t and n_{\parallel} . In particular, 11×8 system with four holes ($n_{\parallel} = 1/2$) definitely forms an edge stripe at $J/t = 0.6$. The same system exhibits a bulk stripe at $J/t = 0.4$. For $J/t = 0.6$, on an 11×8 cluster, we find the following energies per hole for various dopings, in units of t : one hole in the bulk -0.90(1), at the edge -0.94(1); one pair, bulk -1.03(1), edge -1.03(1); $n_{\parallel} = 1/2$ stripe, bulk -1.08(1), edge -1.08(1). Despite the degeneracies for the pair and stripe in the bulk versus the edge, the edge pair and stripe appear quite stable in the DMRG run, and strongly bound to the edge. $J/t = 0.6$ appears to be quite close to the transition between bulk and edge stripes and pairs.

Thus far our DMRG results for the low hole numbers have agreed with the “constrained” analytical results in which only homogeneous hole states were taken into consideration. While this analysis can be directly relevant to certain nano-scale structures doped with few holes, the question remains which phases will survive in the thermodynamic limit. Our energy-per-hole analysis shows that energy is always lower in the stripe phase (bulk or edge). This implies an instability towards a phase separation of a peculiar kind. That is, the system will tend to segregate into a hole empty region and a region where a stripe-like phase will be formed. Gas of pairs (edge or bulk) will not be selected for the ground state. In fact, we observe an indication of such a phase separation already in our t - J_z 11×8 cluster with four holes ($n_{\parallel} = 0.5$). We start at a lower J_z/t with the “regular” bulk stripe which evolves into an excellent edge stripe at larger J_z/t , similar to one in Fig. 3(a). However, on its way to the edge it forms a loop-like stripe object, with clear ADW, attached to the edge with its ends, see Fig. 3(b).

We augmented our study of higher hole concentrations with the 20×5 cluster with open BCs for all the edges and a strong repulsive potential for holes (in the form of a chemical potential $\mu = +t$) along the left, upper, and right edges to create a preferential boundary and look for potential edge states. Hole numbers up to six were studied. They organized themselves into an edge arc-like stripe, see Fig. 3(c). Similar patterns have been produced by four holes as well. Such states show clear signatures of the ADW and are very stable. An “internal” hole concentration per arc unit length can be estimated and is close to $n_{\parallel} = 1/2$. Thus, one can argue that the ground state of the semi-infinite $t - J$ system is likely to be composed of either “straight” or “loop” stripes (depending on a given n_{\parallel}), which attach themselves to the boundary at some J/t . Note, that nowhere in our study a mixed bulk-edge state was detected and, as we discussed, the t - J_z or t - J system with edges should belong to the class described in our Fig. 1(b).

In summary, we have studied the edge phase diagram of a strongly-correlated nano-structure and found that it consists of the bulk pairs, bulk stripes, and edge stripes. Using DMRG and analytical methods we have shown that these edge stripe states are directly related to the bulk stripe states and have their origin in the non-trivial interplay between magnetic and kinetic energies in strongly-correlated systems.

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